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A FINITE DIFFERENCE STUDY OF THE STRETCHING AND BREAK-UP OF FILAMENTS OF POLYMER SOLUTIONS

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ABSTRACT

The stretching and break-up of a viscoelastic filament pulled by a constant weight is studied numerically by a finite difference method. The results show the following tendencies:

- 1. Newtonian filaments, even in the absence of surface tension, show a rapid increase in elongation at one particular point (they "break" there).
- 2. The addition of a viscoelastic polymer prevents or at least delays the break-up, even if it makes only a small difference to shear viscosity.
- 3. Surface tension accelerates break-up, but even in the presence of surface tension elasticity has a stabilizing effect.

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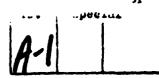
SIGNIFICANCE AND EXPLANATION

Elongational flows of polymeric fluids have received much attention both because of their usefulness in distinguishing reasonable constitutive laws from bad ones and because of their practical importance. A question which if of great practical significance, but is poorly understood, is if and when thin filaments or sheets of a liquid will break-up. This problem arises e.g. in the formation of fibers, in lubrication and in problems involving atomization into droplets. Empirically, it is well known that viscoelastic fluids are much more stable against break-up than Newtonian fluids with comparable viscosity, but an adequate theoretical explanation has so far not been given.

In this paper, we examine a viscoelastic filament, which is attached at the upper end and pulled by a constant weight on the lower end. This problem is motivated by an experiment of J. Matta. The polymer is assumed to satisfy a particular constitutive law known as the "rubberlike liquid". The equations for this problem are formulated and solved by a finite difference method. The results show that Newtonian filaments break up much more easily than viscoelastic filaments. This is the case whether or not surface tension is present. As expected, surface tension accelerates the break-up, but even with large surface tension, the viscoelastic filament is still more stable than the Newtonian one.



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A FINITE DIFFERENCE STUDY OF THE STRETCHING AND BREAK-UP OF FILAMENTS OF POLYMER SOLUTIONS

Peter A. Markowich and Michael Renardy **

1. Introduction

It is well known empirically [1], [2], [7], [9], [10], [13] that filaments of viscoelastic fluids are much more stable against break-up than filaments of Newtonian fluids with comparable viscosity. However, so far this has not been well understood theoretically. Linear stability analysis of uniform jets shows that in fact capillary instabilities should grow faster on a viscoelastic jet than on a Newtonian jet [1], [2], [7], [9]. This has led to the conclusion that the breakup of jets or filaments must be governed by nonlinear effects. However, we are not aware of any precise calculations in the nonlinear regime.

In this paper we study a problem that is motivated by an experiment designed by J. Matta [8] for the measurement of elongational flow properties in dilute polymer solutions. In this experiment, the fluid is slowly extruded from a vertical nozzle and forms a drop at the nozzle tip. As this drop reaches a critical size, it begins to fall and drags a filament behind itself.

We consider the following idealized model problem: A filament is at rest up to time t = 0. For t > 0, one end of the filament is attached (at the "nozzle"), the other is pulled by a constant weight (the "drop"). The visco-

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elastic fluid in the filament is assumed to obey the constitutive law for a "rubberlike liquid" [3], [4], [12].

We use the following notation: x denotes the position of fluid particles in a reference configuration, which may or may not agree with the initial configuration. It is assumed that, in the reference configuration, the filament has uniform radius δ and length 2L, i.e. we have $x \in [-L,L]$. By u(x,t) we denote the spatial position of the particle x at time t. ρ denotes the density of the fluid, η the Newtonian contribution to the viscosity, a the memory function of the rubberlike liquid law, σ the surface tension coefficient, M the mass of the weight, and g the gravitational acceleration. The problem is then described by the following equations (see [11])

(1.1)
$$\rho u_{tt} = \frac{\partial}{\partial x} S[u_x] + \rho g$$

where

(1.2)
$$S[u_{x}] = 3\eta \frac{\partial}{\partial t} \left(-\frac{1}{u_{x}}\right) + \int_{-\infty}^{t} a(t-s) \left(\frac{u_{x}(t)}{u_{x}^{2}(s)} - \frac{u_{x}'s)}{u_{x}^{2}(t)}\right) ds + \frac{\sigma}{\delta} u_{x}^{-1/2}.$$

We have an initial condition:

(1.3)
$$u(x,t) = u_0(x)$$
 , $t < 0$

and boundary conditions

(1.4)
$$u(-L,t) = u_0(-L)$$
 , $t > 0$

(1.5)
$$Mu_{tt}(L,t) = Mg - \pi \delta^2 s[u_X]_{X=L}$$

These equations are discretized by a finite difference method, which is an adaptation of a scheme used earlier on a similar problem [6]. This method is described in section 2.

In section 3 we present numerical results. Particular emphasis is given to the question of: if and when u_x shows catastrophic growth. We shall see that, if the initial thickness is uniform $(u_0(x) = x)$, this always happens at the attached end. The results show that elasticity retards the growth of u_x , while surface tension accelerates it. We give a heuristic explanation of what we believe to be the mechanism for these effects.

2. The discretization scheme

For the discretization of (1.1), we use an implicit Euler scheme in time and symmetric difference approximations in space. This yields a stable scheme which is first order accurate in time and second order accurate in space

[6]. To describe the scheme, we need to introduce some notations.

The grid points are $t_n = nk$, $x_i = ih$ (i = -N, -N+1, ..., N), and approximations to $u(x_i, t_n)$ are denoted by u_i^n . We use the following difference quotients:

(2.1)
$$\Delta^{+}u_{\underline{i}}^{n} = \frac{u_{\underline{i+1}}^{n} - u_{\underline{i}}^{n}}{h}$$

$$\Delta^{-}u_{\underline{i}}^{n} = \frac{u_{\underline{i}}^{n} - u_{\underline{i-1}}^{n}}{k}$$

$$\delta^{+}u_{\underline{i}}^{n} = \frac{u_{\underline{i}}^{n+1} - u_{\underline{i}}^{n}}{k}$$

$$\delta^{-}u_{\underline{i}}^{n} = \frac{u_{\underline{i}}^{n} - u_{\underline{i}}^{n-1}}{k}$$

The discretization of (1.1) is then given by

$$\rho \delta^{+} \delta^{-} u_{i}^{n} = \rho g + 3 \eta \delta^{+} \Delta^{+} \left(-\frac{1}{\Delta^{-} (u_{i}^{n})}\right)$$

(2.2)
$$+ k \sum_{j=-\infty}^{n+1} a(t_{n+1} - t_j) \Delta^{+} \left[\frac{\Delta^{-u_{1}^{n+1}}}{(\Delta^{-u_{1}^{j}})^{2}} - \frac{\Delta^{-u_{1}^{j}}}{(\Delta^{-u_{1}^{n+1}})^{2}} \right]$$

$$+\frac{\sigma}{\delta}\Delta^{+}[(\Delta^{-}u_{i}^{n})^{-1/2}]$$
.

Of course, Δ^+ and Δ^- are interchangeable. For $j \leq 0$, u_1^j is simply $u_0(x_j)$. If a is a finite sume of exponentials, as was always assumed in our calculations, then the sums can be evaluated recursively.

Equation (2.2) has to be supplemented by boundary conditions. These are

$$u_{-N}^{n+1} = u_{0}^{-1}(-L)$$

$$m\delta^{+}\delta^{-}u_{N}^{n} = Mg - \pi\delta^{2}\{3n\delta^{+}(-\frac{1}{\Delta^{+}u_{N}^{n-1}})$$

$$+ k \sum_{j=-\infty}^{n} a(t_{n} - t_{j})[\frac{\Delta^{+}u_{N}^{n}}{(\Delta^{+}u_{N}^{j})^{2}} - \frac{\Delta^{+}u_{N}^{j}}{(\Delta^{+}u_{N}^{n})^{2}}]$$

$$+ \frac{\sigma}{\delta} (\Delta^{+}u_{N}^{n})^{-1/2}\} .$$

Here Δ^* is a second order accurate approximation to u_x :

(2.4)
$$\Delta^* u_N^n = \frac{u_{N-2}^n - 4u_{N-1}^n + 3u_N^n}{2h}.$$

At each time step, (2.2), (2.3) yields a nonlinear system of equations for the u_i^{n+1} , $i=-N,\ldots,N$. This system is solved by Newton's method.

3. Numerical results

In order to test our program, we choose the following parameter values: $L=1, \ \rho=1, \ \eta=10, \ a(t)=e^{-t}, \ \frac{\sigma}{\delta}=1, \ \frac{M}{\pi\delta^2}=1, \ g=1.$ We used the initial condition $u_0(x)=x+\frac{x}{6}$, and we added inhomogeneous terms to (1.1), (1.4) and (1.5) in such a way that $u(x)=x+\frac{x}{6}$ cosh t becomes an exact solution. We obtained the following results at t=5:

h=0.05 k=0.005	u _x	x = -1 -13.27 38.08 -72.78	24.89	14.43	6.95	2.48	1.05	2.48	6.95	14.47	25.04	38.67
h=0.05 k=0.001	u _x	-13.37 38.13 -74.30	24.82	14.38	6.93	2.48	1.04	2.48	6.93	14.38	24.84	38.19
exact	n XX n	-13.37 38.10 -74.21	24.75	-3.27 14.36 -44.53	6.94	2.48	1.0	2.48	6.94	14.36	7.13 24.75 59.37	38.10

The computed solutions are in good agreement with the exact solution. For the following calculations, we chose the mesh sizes k = 0.001, h = 0.05 or less.

We chose parameter values roughly in the range of Matta's experiments, reported in [8]. (All the following numbers are in CGS - units). We picked L=1, $\delta=\frac{1}{10}$ and $u_0(x)=x$, i.e. we start with a uniform filament of length 2 cm and radius 1 mm. We took $\eta=10$, $\rho=1$, $\frac{M}{\pi\delta^2}=10$ and g=20 (in Matta's experiment, the drop falls into another fluid rather than into air). For the surface tension parameter, we chose the values $\sigma=0$, $\sigma=1$ and $\sigma=10$ (the last one is realistic), and for the memory function we used a=0, $a=e^{-t}$ and $a=10e^{-t}$. It should be noted that $a=e^{-t}$ increases the shear viscosity by only 10%, while $a=10e^{-t}$ doubles it.

The computed results for the Newtonian fluid show a pronounced boundary layer at x = -1. This is illustrated by Figure 1, which was obtained for $\sigma = 0$, h = 0.05 and k = 0.001. As would be expected, the effect of the discretization is to diminish the rapid growth of u_X and the real values for $u_X(-1)$ are even larger. This is illustrated by the following table, which compares values of $u_X(-1)$ and $u_{XX}(-1)$ for two different values of h:

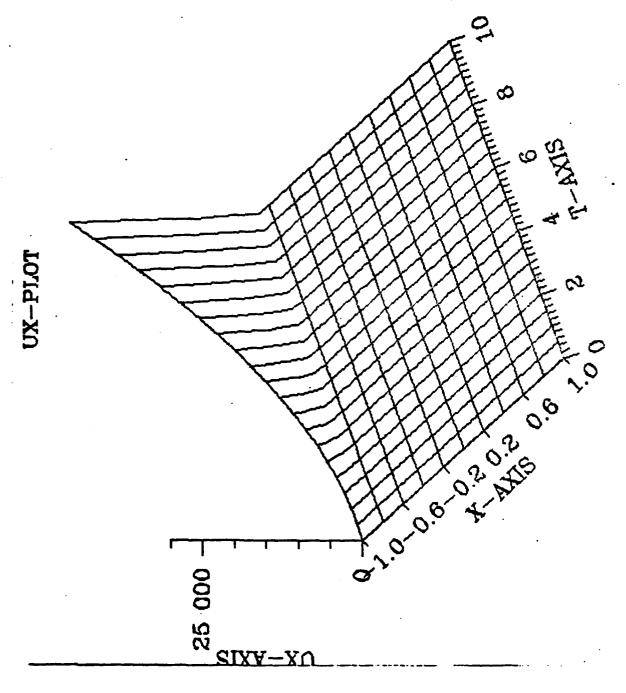


Figure 1

		h = 0.05		h = 0.005			
t	u _x (-1)	u _{xx} (-1)	$\frac{u_{xx}}{u_x^2t}$	u _x (-1)	u _{xx} (-1)	$\frac{u_{xx}}{u_{x}^{2}t}$	
0.5	3.34	-3.62	-0.65	3.35	-3.75	-0.67	
0.6	5.02	-9.47	-0.63	5.06	-10.21	-0.66	
0.7	7.84	-25.19	-0.59	8.01	-29.85	-0.66	
0.8	12.68	-66.07	-0.51	13.38	-94.63	-0.66	
0.9	20.81	-162.94	-0.42	23.65	-326.42	-0.65	
1.0	33.85	-362.52	-0.32	44.23	-1201.38	-0.61	

The second column shows a more rapid growth of u_x and in particular of u_{xx} . The quantity $\frac{u_{xx}}{u_x^2t}$ should theoretically be independent of t, as one can easily deduce from the equation. Away from x = -1, the computed values are almost identical. We believe it is likely that, in fact, the values of $u_{xx}(-1)$, $u_x(-1)$ tend to infinity in finite time, but it would take rather strong mesh refinements to verify this numerically.

As expected, the presence of surface tension accelerates the growth in the boundary layer. The following table shows some computed values of $u_{\chi}(-1)$ and $u_{\chi}(-0.8)$ (h = 0.005, k = 0.001):

	σ = 0		σ:	= 1	σ = 10		
t	u _x (-1)	u _x (-0.8)	u _x (-1)	u _x (-0.8)	u _x (~1)	u _x (-0.8)	
0.5	3.35	2.80	3.35	2.77	3.38	2.48	
1.0	44.23	9.62	65.63	9.20	1731.19	1.37	
1.5	906.72	16.11	2372.01	11.96	4791.56	0.35	
2.0	3980.76	20.50	8108.24	9.43	9085.79	0.16	

The table shows that the effect of surface tension at $\sigma=1$ is relatively slight, but is large at $\sigma=10$ (a realistic value).

Elasticity has the effect of smoothing out the boundary layer and delaying the rapid growth of $u_{\chi}(-1)$. The following talbe shows computed values for $u_{\chi}(-1)$, $u_{\chi}(-0.8)$ at t = 1 (h = 0.005, k = 0.001):

	σ = 0		σ:	- 1	σ = 10	
	u _x (-1)	u _x (-0.8)	u _x (-1)	u _x (-0.8)	u _x (-1)	u _x (-0.8)
a(t) = 0	44.23	9.62	65.63	9.20	1731.19	1.37
a(t) = e-t	23.38	10.29	26.53	10.21	68.78	3.51
a(t) = 10e-t	9.63	8.30	9.79	8.36	13.07	9.9

We can clearly see that even small amounts of elasticity have a substanti 1 stabilizing influence.

An interesting feature arises in the case $a(t) = e^{-t}$, $\sigma = 1$ (Figure 2). We see a step in the surface at approximately x = -0.1. In fact, the computed values at t = 10 are $u_x(-0.2) = 478.43$, $u_x(0.0) = 1.74$. Roughly half the filament (x < -0.1) is stretching, while the other half is actually shrinking and ultimately absorbed into the drop. This sort of feature does not occur if surface tension is absent.

A key to a qualitative understanding of the mechanism governing these results may be in results found by Petrie [10] and Renardy [5], [11]. They discuss stretching of a filament of uniform thickness with no inertia. The filament is stretched by a force pulling the ends. In the Newtonian case the length of the filament can reach infinity in finite time, even for a finite force. This is because the filament gets weaker as it gets thinner, and there can be a catastrophic growth. Elasticity of the fluid opposes this, and for the model studied here, a blow-up is impossible.

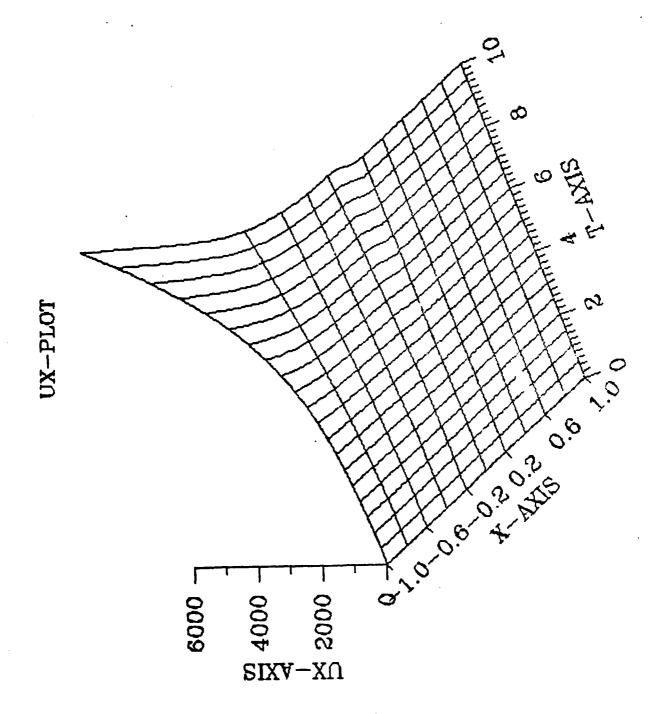


Figure 2

In the present situation, the stretching of the filament is very inhomogeneous and this is mostly due to the influence of gravity. The filament "wants" to fall, but is prevented from doing so at x = -1. Thus, it stretches most rapidly at this particular point. Our results show a qualitative similarity to those mentioned above: In the Newtonian case we find catastrophic growth at the weakest point of the filament. Elasticity suppresses or at least delays this effect.

In the previous calculations, breaking of the filament always took place at x = -1. In experiments, this is usually not the case for two reasons:

- The filament is not really "attached" at the upper end. Instead, fluid is still supplied from the nozzle.
- The assumption of a homogeneous filament as initial state is not realistic.

We did some calculations with the initial value $u_0(x) = 1.25x - 0.25x^3$, corresponding to a filament that is thinner in the middle. Otherwise we used the same parameters as above. The following table shows the values of u at t=2 for a Newtonian filament and $\sigma=0$ and 10 (the step sizes are again h=0.005, k=0.001):

×	$u(x,t=2), \sigma = 0$	$u(x,t=2), \sigma = 10$
-1	-1.00	-1.00
-0.8	-0.21	-0.98
-0.6	7.22	-0.95
-0.4	17.97	-0.92
-0.2	26.30	-0.85
0	31.75	29.10
0.2	34.86	29.14
0.4	36.50	29.17
0.6	37.37	29.19
0.8	37.83	29.21
1.0	38.06	29.23
	1	· ·

The second column shows that the filament breaks somewhere between x = -0.2 and x = 0.

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19. KEY WORDS (Continue on reverse eide if necessary and identify by block number)

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